

LETTERS TO THE EDITOR

The Letters to the Editor section is divided into three categories entitled Notes, Comments, and Errata. Letters to the Editor are limited to one and three-fourths journal pages as described in the Announcement in the 1 July 2003 issue.

ERRATA

Erratum: “Photodissociation of LiFH and NaFH van der Waals complexes: A semiclassical trajectory study” [J. Chem. Phys. 115, 7945 (2001)]

Ahren W. Jasper, Michael D. Hack, Arindam Chakraborty, and Donald G. Truhlar

*Department of Chemistry and Supercomputing Institute, University of Minnesota,
Minneapolis, Minnesota 55455*

Piotr Piecuch

Department of Chemistry, Michigan State University, East Lansing, Michigan 48824

[DOI: 10.1063/1.1615236]

An error has been discovered in the computer program that was used to simulate photodissociation initial conditions. This error caused a significant number of trajectories to have high-energy initial geometries corresponding to unphysical bend angles. The resulting dynamics, therefore, does not accurately reflect the photodissociation dynamics out of the ground vibrational state of the van der Waals complex as indicated in the paper. We have corrected this error,

and the corrected results are given in Tables I and II. Note that using the corrected sampling scheme, the range of excitation energies is limited to 1.3–1.58 eV and 1.7–1.9 eV for LiFH and NaFH, respectively.

The corrected results differ qualitatively from the published results, but the main conclusion of the paper (that the lifetime of the LiFH complex is shorter and less sensitive to excitation energy) is still valid.

The authors are grateful to Jill E. Leas for carrying out the new calculations with the corrected computer program.

TABLE I. Corrected results for NaFH.

Method	$h\nu$ (eV)	τ (ps)	P_R	$\langle v' \rangle$	$\langle j' \rangle$	P_Q	$\langle v'' \rangle$	$\langle j'' \rangle$
NDMa	1.70	3.0	0.76	2.96	14.2	0.24	1.54	8.1
	1.75	1.8	0.80	2.89	14.4	0.20	1.60	8.7
	1.80	1.0	0.85	2.69	14.6	0.15	1.78	8.1
	1.85	0.60	0.88	2.80	15.0	0.12	1.93	8.7
	1.90	0.43	0.86	3.06	15.9	0.14	8.97	9.0
TFSa	1.70	2.5	0.93	3.35	13.0	0.07	2.08	10.5
	1.75	1.4	0.94	3.77	12.9	0.06	2.06	12.3
	1.80	0.81	0.96	3.90	13.6	0.04	2.11	12.9
	1.85	0.42	0.97	4.06	14.2	0.03	2.19	12.0
	1.90	0.37	0.97	4.48	14.8	0.03	2.12	11.9
NDMd	1.70	0.34	0.34	2.69	15.4	0.66	0.74	9.9
	1.75	0.27	0.50	3.04	16.6	0.50	1.00	9.6
	1.80	0.24	0.62	3.38	17.1	0.38	1.16	9.3
	1.85	0.20	0.72	3.60	17.4	0.28	1.31	9.6
	1.90	0.19	0.73	4.02	19.4	0.27	1.50	8.9
TFSd	1.70	0.19	0.71	1.30	15.8	0.29	2.04	5.2
	1.75	0.10	0.82	1.83	16.5	0.18	2.16	5.1
	1.80	0.027	0.89	2.61	16.8	0.11	2.29	5.0
	1.85	0.028	0.91	3.67	16.9	0.09	2.25	5.8
	1.90	0.035	0.92	4.08	17.9	0.08	2.22	5.9

TABLE II. Corrected results for LiFH.

Method	$h\nu$ (eV)	τ (ps)	P_R	$\langle v' \rangle$	$\langle j' \rangle$	P_Q	$\langle v'' \rangle$	$\langle j'' \rangle$
NDMa	1.30	0.41	0.88	1.77	6.3	0.12	1.33	3.0
	1.40	0.13	0.90	2.20	6.5	0.10	1.53	3.5
	1.50	0.073	0.91	2.46	12.2	0.09	1.25	8.7
	1.58	0.092	0.96	2.09	15.7	0.04	1.09	11.1
TFSa	1.30	0.43	1.00	2.16	6.7	0.00	1.31	10.0
	1.40	0.22	0.99	2.32	6.8	0.01	1.92	6.3
	1.50	0.086	1.00	1.95	5.9	0.00	2.00	10.5
	1.58	0.12	1.00	2.06	10.1	0.00	2.00	8.0
NDMd	1.30	0.14	0.61	2.65	9.9	0.39	0.68	5.6
	1.40	0.089	0.75	3.09	8.7	0.25	0.95	3.9
	1.50	0.054	0.93	2.98	7.6	0.07	1.21	3.7
	1.58	0.034	0.99	2.17	16.5	0.01	1.50	6.5
TFSd	1.30	0.031	0.85	2.12	7.4	0.15	1.21	4.4
	1.40	0.020	0.95	3.35	7.6	0.05	1.61	3.6
	1.50	0.016	0.96	3.93	7.4	0.04	1.44	3.8
	1.58	0.030	0.86	3.37	10.0	0.14	1.43	5.5